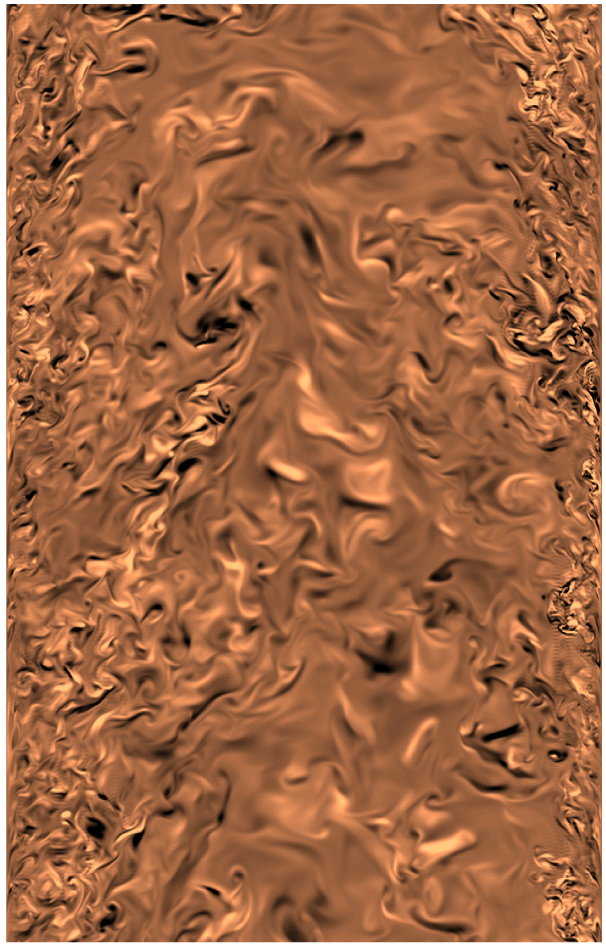
ALCF Early Science Program

Argonne NATIONAL LABORATORY

Petascale Direct Numerical Solutions of Turbulent Channel Flow

ESP Kick-Off Workshop and Project Plan Presentation



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Outline

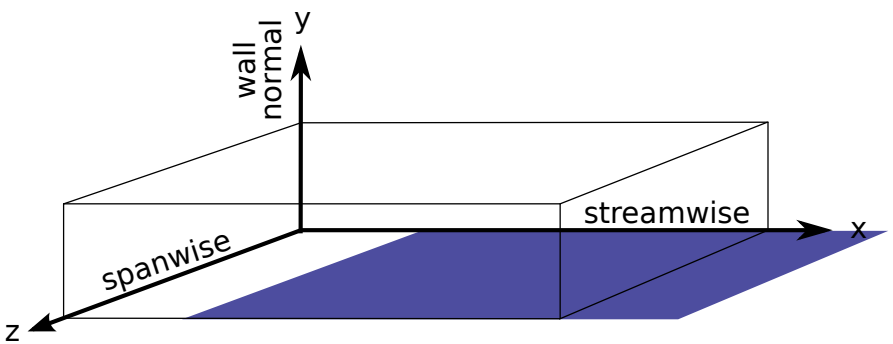
Project Overview

Turbulent Fluid Flow

- 28% of annual USA energy consumption is used for transportation
  - Wall-bounded fluid flows: car, plane wing, pipes, etc.
  - Turbulent skin friction: dominant cause of energy loss
- Efforts to reduce drag are impeded by lack of accurate models

Direct Numerical Simulations (DNS)

- Resolves all scales – no modeling
- Cost increases as Re^3
- Target: turbulent channel DNS
  - $Re_\tau \approx 5000$
  - (16384,1024,12288) grid



Numerical Method

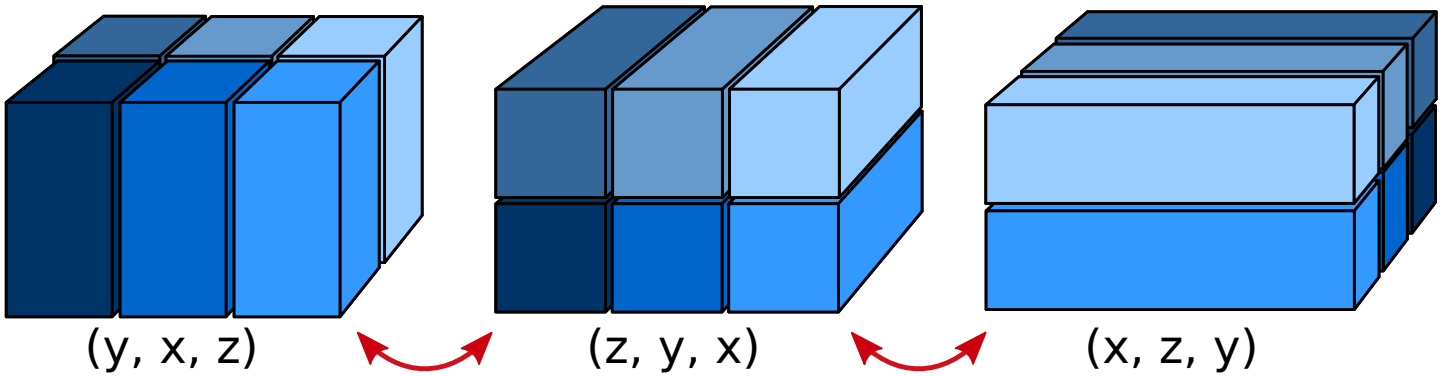
- Unsteady, incompressible Navier-Stokes equations (KMM, 87)

$$\frac{\partial u_i}{\partial t} = -\frac{\partial P}{\partial x_i} + H_i + \frac{1}{Re}\nabla^2 u_i \tag{1}$$

- Fourier spectral in spanwise and streamwise directions
- Compact finite difference in the wall normal direction (Lele, 91)
- Partially implicit third-order Runge-Kutta/Crank-Nicholson scheme for time stepping (Spalart et al, 91)

Parallelism

- Fortran90 + MPI
- Structured grid – “Pencil” decomposition



I/O Requirements

- ESIO: parallel HDF-5
- $8 \times 3 \times N_y N_x N_z \approx 6.6$ TB per file
- Write frequency approximately one per wall clock hour
  - Writing ≈ 350
  - Archiving ≈ 100

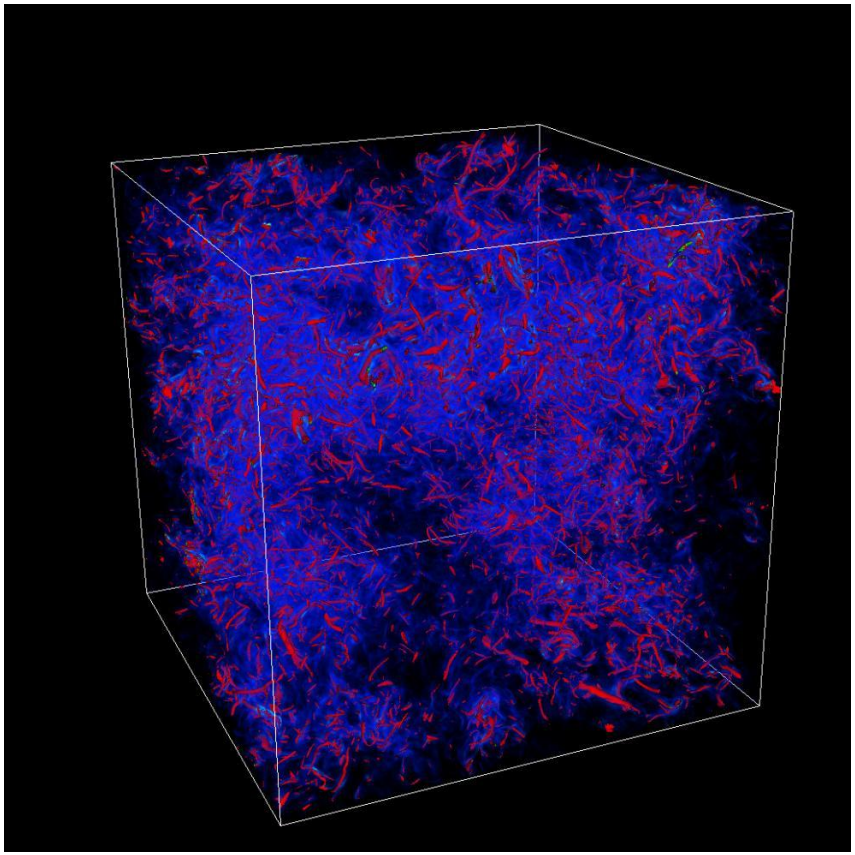
Software Dependencies

Libraries:

- FFTW3/ESSL
  - P3DFFT
- BLAS
- LAPACK
- pHDF-5

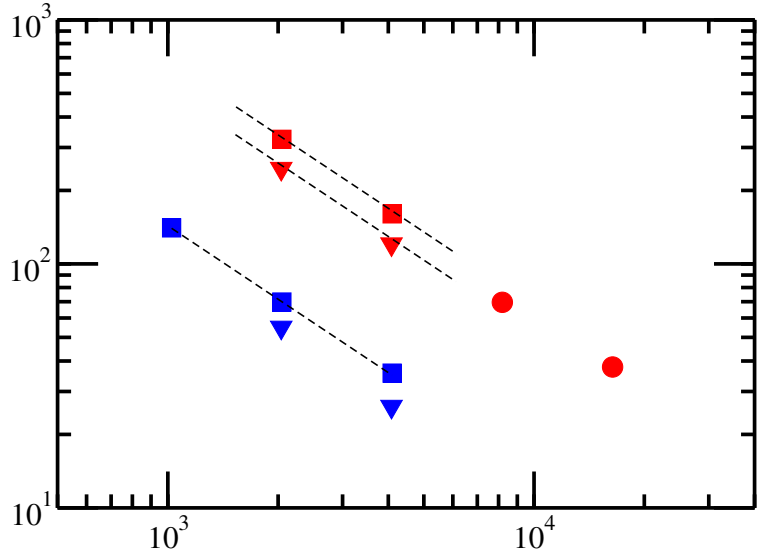
Tools:

- ParaView/VisIT



Performance and Scaling

- (12288,901,9216)
  (6144,633,4608)
- Strong scaling: 8k to 32k cores
- Target:
  - (16384,1024,12288) grid
  - 12 flow through times
  - 1.2 M time steps



Anticipated Modifications for Blue Gene/Q

- openMP – node-level parallelism
- B-spline capability
- I/O tuning

Six Month Plan

- Find and hire a project postdoc
- Detailed performance measurements on Blue-Gene/P
- OpenMP
- I/O kernel tuning / integration
- ESSL/FFTW
- Start smaller runs:
  - (4096,256,3072), 8 flow through, 50k hours
  - (8192,512,6144), 4 flow through, 5M hours

..and beyond

- Overlap computation/communication
- Fault tolerance
- Asynchronous I/O

Thank you!

Questions?

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